

## **Minutes of**

# The 10<sup>th</sup> MIRAGE Meeting

Monday 24<sup>th</sup> June, 2019

**Dom Hotel Limburg** Limburg, Germany

> 8 August, 2019 Dr. Carsten Kettner



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These minutes summarizes the conclusions, decisions and results from the 10<sup>th</sup> MIRAGE meeting which took place at Dom Hotel Limburg, Germany, on Monday, 24 June, from 9 am to 5 pm.

Any further information about the MIRAGE project is available at the project website, i.e. <u>https://www.beilstein-mirage.org</u>

#### The Agenda

At the Boston MIRAGE meeting, August 2018, we agreed on a comprehensive tasklist. Thus, in a first approximation, status reports and content-related discussions will make the major part of our program.

#### Monday, 24 June

9.00	Welcome and Opening - CK		
	MIRAGE – an overview - CK		
	<ul><li>Wikipedia entry</li><li>Website</li><li>Flyer</li></ul>		
	Tasks agreed at the Boston MIRAGE meeting:		
	<ul> <li>Status and Discussions + Outlook</li> <li>Making guidelines "useful" (templates, etc.) <ul> <li>LC Guidelines - MC</li> <li>CE Guidelines - JZ</li> <li>Glycan reagents specificity Guidelines - JP</li> <li>Glycopeptide Analysis Guidelines - FL</li> <li>Lectin Array Experiments Reporting Guidelines - JP</li> </ul> </li> </ul>		
	NMR Guidelines – JP, JJB, AMC		
	Overview, drafting, strategy		
12.30	Lunch		
	Promotion with Journals		
	<ul> <li>In general: Glycobiology, PLOS, Carbohydrate Res., Glycoconjugate J. Mol. Omics (TF, DK, FL, NP, JP)</li> <li>In particular, for Glycan Microarrays: PNAS, Nature, JBC, etc. (TF, JP)</li> </ul>		





	Further advancing the MIRAGE guidelines in the community Short presentations of MIRAGE related spin-off projects welcome!	
	Ontologies and Metadata	
	<ul> <li>Status and discussions</li> <li>Individual ontologies vs. one-in-all</li> <li>Data exchange formats?</li> </ul>	
	MC, FL, RR, KAK	
17.00	Summary and Close	
19.30	Welcome Reception Beilstein Glyco-Bioinformatics Symposium 2019	

#### List of Participants (as of May 2019)

- 1. Kiyoko Aoki-Kinoshita, Soka University Tokyo, Japan
- 2. Matthew Campbell, Griffith University, Gold Coast/Brisbane, Australia
- 3. **Maria Angeles Canales**, Complutense University of Madrid, Spain
- 4. **Catherine Costello**, Boston University, Boston, MA, USA
- 5. **Ten Feizi,** Imperial College London, UK
- 6. **Niclas Karlsson**, Gothenburg University, Gothenburg, Sweden
- 7. **Carsten Kettner**, Beilstein-Institut, Frankfurt am Main, Germany
- 8. **Frédérique Lisacek**, SIB Swiss Institute of Bioinformatics, Geneva, Switzerland
- 9. Nicolle Packer, Macquarie University, Sydney, Australia



- 11. René Ranzinger,
  University of Georgia, Athens, GA, USA
  12 Weston Struwo
- 12. Weston Struwe, Oxford University, Oxford, UK
- 13.**Rob Woods**, University of Georgia, Athens, GA, USA
- 14. **Joe Zaia**, Boston University, Boston, MA, USA





#### 10. James Paulson,

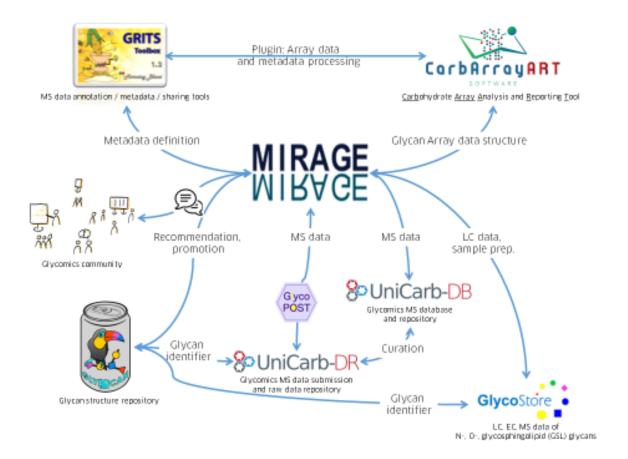
The Scripps Research Institute, La Jolla, CA, USA

#### **Status and Progress**

#### Overview

Since the last meeting held in Boston in August 2018, the MIRAGE project has made reasonable progress and many of the tasks negotiated there have been started and developed by the MIRAGE members in charge.

First, CK gave an overview of the status of those tasks he is responsible for and started with the overall MIRAGE landscape that considers the MIRAGE project a hub or platform for discussing and promoting exchange formats, standards and networking for repositories, databases and software tools.



In a retrospective, it has not been anticipated that MIRAGE would take this direction but the outcome fits very well with the statement from 2006 that "the scientific community agreed to establish a worldwide linked electronic infrastructure for the storage and



analysis of carbohydrate structure data. As a prerequisite, standardized protocols were proposed for the exchange and the publication of experimental data and metadata" (Packer et al., 2008; PMID:18095367). However, it became clear that the aims proposed on the project's website need some extending statements or they need to be broadened in a general way.

The subsequent discussion has addressed some aspects but no final decision has been made. As the modification of the aims need to be worked out in more details it has been agreed to postpone this discussion to another meeting. Finally, there is general consensus that the websites need to be updated (see task list for details).

#### Wikipedia entry

FL and CK succeeded in publishing information about the MIRAGE project on the English pages of Wikipedia. Here, MIRAGE is part of the Minimum Information Standards main page and the access to the MIRAGE entries is here: https://en.wikipedia.org/wiki/

Minimum\_Information\_Required\_About\_a\_Glycomics\_Experiment.

In order to find "our" MIRAGE article more quickly, it is suggested to make a corresponding entry on the "Disambiguation" page.

Maybe, the "Glycobiology" chapter could be extended by a paragraph on reporting guidelines for glycobiology experimental data. It's worth a try this addition and to see whether this entry will be accepted by the Wikipedia team and thus be stable.

#### **MIRAGE Flyer**

CK presented the latest draft version of the MIRAGE flyer. This draft has been generally accepted but it was requested to send this version to the members of the Commission for the final review (details, see task list). The flyer will be then finalized and printed. A reasonable number of copies will be sent to the members of the MIRAGE Commission for further dissemination on conferences, in departments etc. to raise more awareness within the community.

#### Guidelines

#### LC Guidelines

The LC Guidelines have been made public on the project's website in March 2019 and published in Glyobiology on 26 March, 2019 (Volume 29, Issue 5, May 2019, Pages 349–354, https://doi.org/10.1093/glycob/cwz009). Examples for experimental results applying LC for the analysis of glycans can be found on the MIRAGE website





("Examples"). In accordance to the Glycan microarray guidelines the generation of both a template and a completed example has been suggested.

#### **CE Guidelines**

With the demission of Franklin Leach due to other commitments JZ took over, again and he will proceed with the manuscript on the basis of an old version.

JZ will contact Manfred Wuhrer for support.

Update: in July, CK asked Erdmann for the most current version of both the draft of the CE Guidelines and the corresponding manuscript as CK has none of it available.

#### Glycan reagents specificity Guidelines

JP reported the results of his studies on the relevance of such guidelines. From audio meetings he draws the conclusion that such guidelines seem to be very hard to specify as this field appears very diverse and may interfere with potential guidelines for reporting lectin specificity experiments. Thus, JP suggested to refocus on the aims initially in mind and to rename this task into "*Glycan binding protein specificity*" guidelines which also may include antibodies. He has identified a number of scientists interested in this topic including Lara Mahal.

#### **Glycopeptide Analysis Guidelines**

FL reported that the representation of glycopeptides is by far more diverse than initially anticipated and thus she has underestimated the efforts required to be able to present a first draft. For example, there are uncertainties on the representation of glycan compositions attached with peptides. There were a number of suggestions that are intended to support FL in rethinking this task including questions how the data have been obtained. In addition, the draft of a data generation workflow (comparable with that from the glycan microarrays) is considered an option to create a scaffold for future guidelines. Finally, it was suggested to first have a generic guideline document followed by a subsequent document that defines formats and orders of the composition of glycopeptides.

#### Lectin Array Experiments Reporting Guidelines

After a conference call with Lara Mahal and Hiroaki Tateno the idea has emerged to use the Glycan array Guidelines as a template. In addition, in order to address the more general nature and being more consistent with the aims of the Glycan reagents specificity Guidelines it was suggested to rename this task into "*Carbohydrate binding protein array Guidelines*".



#### NMR reporting Guidelines

Angeles Canales presented a first draft of NMR Reporting Guidelines which have been defined in collaboration with JP and Jesús Jiménez-Barbero and is actually split into two separate guidelines each for free and bound glycans.

#### Promotion with Journals

As agreed some members of the MIRAGE Commission are in contact with a number of journals. TF and JP are in contact with the editor-in-chief of *Glycobiology*, Robert Haltiwanger who is interested in supporting the MIRAGE Guidelines, in particular the Glycan array guidelines by extending the submission system by a checkbox which asks the submitting author whether his data are compliant with the MIRAGE Guidelines if relevant. In addition, TF and JP succeeded in adding the Glycan array guidelines to the requirements of *MCP*. TF is in close contact with an editor at *Nature* and she is waiting for a decision on the inclusion of the MIRAGE guidelines in the list of guidelines recommended by *Nature*. TF and JP developed a letter template which could be used with some modifications for the first contact of all journals.

DK is in close contact with *Glycoconjugate Journal* and when in charge he insists the authors to consider the MIRAGE Guidelines when reporting relevant experimental data. NP became in charge as guest editor of *Mol. Omics* and is organizing a special issue. Here, she also will recommend the authors to refer to the MIRAGE guidelines where relevant.

FL is in contact with *PLOS* as she is member of the editorial board of *PLOS One*. However, progress is slow from experience.

CK suggested to contact *Scientific Data* and to make GlytouCan, UniCarb-DR and GlycoPost recommended repositories for glycan data. This suggestion has been accepted.

#### **Ontologies and Metadata**

The MIRAGE MS guidelines are currently used in UniCarb-DR and GlycoPOST as Excel files, for which a template was created at the MIRAGE meeting in Sapporo. However, a separate bioinformatics group meeting is needed to finalize the ontologies and



controlled vocabularies to use in these systems. In particular, an exchange format for glycoconjugates is greatly needed as technologies to characterize glycoconjugates are increasingly being developed in the community. The HELM format is one representation that could be of interest for the community; the developers of HELM are in fact currently developing a way to incorporate glycans into their representation format.

#### Tasklist

Task	Responsibility (lead)
<ul> <li>MIRAGE @ Wikipedia</li> <li>Get Wiki page into https://en.wikipedia.org/wiki/Mirage_(disambiguation)</li> </ul>	F. Lisacek
<ul> <li>MIRAGE Website:</li> <li>Updates required, status sections with outdates timestamps, landscape figure on the landing page, guidelines added to this figure, add twitter hashtag to news box, dead links to be replaced, all group pictures on website,</li> <li>Redefinition of aims to be postponed.</li> </ul>	C Kettner
<ul> <li>MIRAGE Flyer</li> <li>Send to final review to Commission, share as link for everybody to share (Downloads)</li> </ul>	C. Kettner
LC Guidelines <ul> <li>Provide template and completed example</li> </ul>	M. Campbell
<ul> <li>CE Guidelines</li> <li>Contact Manfred Wuhrer</li> <li>CK sends CE files to JZ,</li> <li>Review of Guidelines and first draft of manuscript</li> </ul>	J. Zaia
<ul> <li>Glycan reagents specificity Guidelines</li> <li>Renamed to Glycan Binding Protein Specificity</li> <li>First draft at next MIRAGE Meeting</li> </ul>	J. Paulson
<ul> <li>Glcopeptide Analysis Guidelines</li> <li>Draft of generic guidelines,</li> <li>Definition of formats/orders of composition</li> <li>First draft in September at the HUPO Meeting</li> </ul>	F. Lisacek





Task	Responsibility (lead)
<ul> <li>Lectin Array Reporting Guidelines</li> <li>Renamed to Carbohydrate- (Glycan-)Binding Protein Array</li> <li>Revision latest by next meeting</li> </ul>	J. Paulson
<ul> <li>Array Guidelines (in general)</li> <li>Review these guidelines for application with other technologies such as bead array, Next Gene Sequencing etc.</li> <li>Contact groups applying/involved in these techniques</li> </ul>	R. Ranzinger
<ul> <li>NMR Guidelines</li> <li>Revision</li> <li>Contact Kato, Peters, Mulloy, Widmalm for checking revised version</li> </ul>	J. Paulson, A. Canales
Intact Glycoproteins Guidelines <ul> <li>First draft at next meeting</li> </ul>	W. Struwe
<ul> <li>Promotion with journals</li> <li>JPR to adopt Guidelines</li> <li>Nature</li> <li>Letter template to Commission (requires modifications for the corresponding needs)</li> <li>PLOS (One and other)</li> <li>Mol. Omics (in particular special issue)</li> <li>JACS (L. Kiessling) via Jesús Jiménez-Barbero</li> <li>JBC (via Gerry Hart)</li> <li>ACS Chemistry Central Science via C. Bertozzi</li> </ul> Recommended Repository <ul> <li>Contact Scientific Data to make them aware of at least three repositories for glycan data, i.e. GlyTouCan, Unicarb-DR, Glyco-POST</li> </ul>	J. Paulson J. Paulson, T. Feizi J. Paulson, T. Feizi F. Lisacek N. Packer A. Canales C. Kettner J. Paulson C. Kettner
<ul> <li>Unicarb-DR, Glyco-POST</li> <li>These repositories should be added to list of recommended repositories which is effective for all Springer-Nature journals</li> </ul>	
<ul> <li>Ontologies and Metadata</li> <li>Drafts for glycan arrays, MS, LC, and Sample Prep</li> <li>Strategy either for one-in-all or for separate ontologies</li> </ul>	M. Campbell F. Lisacek R. Ranziner K. Aoki-Kinoshita N. Karlsson